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A Steady-State Reaction-Diffusion Problem in a Moving Medium

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We examine a mathematical formulation of the problem of a thin rod held against a source of chemical which diffuses into the rod and reacts with it. The velocity of the rod, which occurs as a coefficient in a coupled system of differential equations, is not known *a priori* but is to be determined as part of the solution.

INTRODUCTION

Consider a thin rod of a chemical W lying along the positive x-axis and fed to the left against a constant source of reactant U located at the origin. The chemical U both diffuses into the rod and reacts with it; the material of the rod does not diffuse. We assume that the reaction of U and W goes to completion in finite time and we postulate that the rod is fed to the left as fast as the end of the rod at the origin is consumed in the reaction, say with velocity v. This corresponds to keeping the end of the rod pressed against a grating located at $x=0$. Since we shall consider only the steady state, v is a constant. The magnitude of this velocity is not known initially, but is to be determined as part of the problem. Allowing for the fact that U is diffusing into a moving medium [2], a suitable prototypical pair of reaction-diffusion equations for a model of this problem are

$$u''(x)+vu'(x)=ku^{\alpha}(x)\,w^{\beta}(x) \tag{1}$$

$$vw'(x)=u^{\alpha}(x)\,w^{\beta}(x), \tag{2}$$

where u and w are the normalized concentrations of U and W, respectively. We assume at first that the motion of the infinitely long rod is controlled by a feeding and wiping device located at $x=X$; this mechanism removes

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any reactant U that reaches that point. Thus suitable boundary data for this finite-length problem are

$$\begin{aligned} u(0)&=1, \qquad & u(X)&=0 \\ w(0)&=0, \qquad & w(X)&=1 \end{aligned} \tag{3}$$

with the further requirement that $w(x)>0$ for $x>0$; this latter is the condition that the rod is fed as rapidly as it is consumed. Later we examine the case of the semi-infinite rod.

If $\beta \geqslant 1$, then the right-hand side of (2) is Lipschitz in w; with u determined, (2) plus the initial condition $w(0)=0$ forces $w \equiv 0$ by the usual uniqueness theorem. Therefore we must have $0<\beta<1$; *we assume* $0<\beta<1$ *throughout the following analysis*. This condition on β is well known to correspond in general to the possible existence of a dead core [6] in W, i.e., of a region in which the concentration of W is zero while the concentration of W is not everywhere zero. Thus it is the phenomenon of the existence of a dead core in W that makes the problem we consider possible.

The problem (1)–(3) is nonstandard in that a coefficient in the differential equation is a priori unknown and the number of boundary conditions exceeds by one what would otherwise be expected. Thus (1)–(3) has points of similarity with inverse problems, as well as with moving-boundary problems. The problem we consider was directly inspired by the papers [1, 3].

The problem (1)–(3) also arises in a slightly different context. Consider the nonlinear system of time-dependent reaction-diffusion equations for a fixed medium:

$$\begin{aligned} -U_t(z,t)+U_{zz}(z,t)&=kU^\alpha(z,t)\,W^\beta(z,t) \\ -W_t(z,t)&=U^\alpha(z,t)\,W^\beta(z,t) \end{aligned}$$

(the chemical of concentration W does not diffuse). If we look for a traveling-wave solution of the form $U(z,t)=u(z-vt)$, $W(z,t)=w(z-vt)$ we obtain (1)–(2) on setting $x=z-vt$. Thus our problem amounts to seeking a finite traveling wave of a specified shape—one satisfying the boundary conditions (3)—to the system of equations above. For a study of traveling-wave solutions to a single diffusion-reaction equation, see [5] and the references given there.

On physical grounds, by a solution of (1)–(3) we shall understand a triple (u, v, w) with $u \in C[0, X] \cap C^2(0, X)$, $u \geqslant 0$, $v>0$, $w \in C[0, X] \cap C^1(0, X)$, $w \geqslant 0$ such that (1)–(2) are satisfied on $(0, X)$ and (3) is satisfied on the boundary. Thus we shall be concerned only with nonnegative solutions.

We first consider a special case, corresponding to the limit $\alpha \downarrow 0$. This special problem is not only interesting in its own right because it can be solved in essentially closed form, but a similar argument is the basis of our proof of existence for the general case. Next we use suitable a priori estimates and the topological transversality theorem [4] to establish existence of solutions of (1)–(3). Uniqueness of solutions of the problem is shown next. Incidental to uniqueness but vital for subsequent considerations, we show that the velocity v is a nondecreasing function of rod length X. Then we show that a dead core in U exists when $\alpha < 1$ and X is sufficiently large; this section was inspired by the problem treated in [3]. Finally, we extend our results to the case of a semi-infinite rod.

Hypotheses throughout the remainder are $0 \leqslant \alpha$, $0 < \beta < 1$, and $w(x) > 0$ for $x > 0$.

The Special Case $\alpha = 0$

The equations we want to examine are

$$u''(x) + vu'(x) = k\,|w(x)|^{\beta}\,\mathrm{sgn}\,u(x) \tag{4}$$

$$vw'(x) = H(|u(x)|)\,|w(x)|^{\beta}, \tag{5}$$

where $H(z) = 1$ if $z > 0$, $= 0$ if $z \leqslant 0$ is the Heaviside function; since we shall show that any solution of these equations with the boundary conditions (3) necessarily satisfies $u \geqslant 0$, $v > 0$, $w \geqslant 0$, any solution of this problem will also be a nonnegative solution of (1)–(3) for $\alpha = 0$. Since (5) implies that $w' \geqslant 0$, we have $0 < w \leqslant 1$ on $(0, X]$. Were u anywhere negative, there would exist a point $\zeta \in (0, X)$ such that $u(\zeta) < 0$, $u'(\zeta) = 0$, and $u''(\zeta) \geqslant 0$; but this contradicts (4). Hence $u \geqslant 0$. If u had a strict local maximum at $\theta \in (0, X)$, then $u'(\theta) = 0$ and there would exist some interval $(\theta, \phi]$ on which $u(\theta) > u(x) > 0$ held. From (4) we obtain that $u''(x) + vu'(x) > 0$ on $(\theta, \phi]$, which implies that $u'(x) - u'(\theta) \geqslant v[u(\theta) - u(x)] \geqslant 0$ there, clearly an impossibility. Therefore u is nonincreasing.

The remainder of our considerations split into two cases depending on whether $u(x) = 0$ somewhere in $(0, X)$.

Case 1. $u(x) = 0$ for some $x \in (0, X)$. In this case let ξ denote the least x for which $u(x) = 0$. Then from (5) we have that

$$\frac{vw^{1-\beta}(x)}{1-\beta} = \begin{cases} x, & 0 < x < \xi \\ \xi, & \xi \leqslant x < X. \end{cases}$$

Set $x = X$ to obtain that $v = (1-\beta)\xi > 0$; then

$$w(x) = \begin{cases} (x/\xi)^{1/(1-\beta)}, & 0 < x < \xi \\ 1, & \xi \leqslant x < X. \end{cases}$$

Now (4) becomes

$$u''(x)+(1-\beta)\,\xi u'(x)=\begin{cases}k(x/\xi)^{\beta/(1-\beta)}, & 0<x<\xi\\ 0, & \xi\leqslant x<X.\end{cases}$$

An integration and continuity of u and u' at ξ imply that

$$u'(x)+(1-\beta)\,\xi u(x)=\begin{cases}k(1-\beta)\,\xi((x/\xi)^{1/(1-\beta)}-1), & 0<x<\xi\\ 0, & \xi\leqslant x\leqslant X.\end{cases}$$

Further integration yields

$$e^{(1-\beta)\xi x}u(x)=1+k(1-\beta)\xi\int_0^x\left(\frac{t}{\xi}\right)^{1/(1-\beta)}e^{(1-\beta)\xi t}\,dt-k(e^{(1-\beta)\xi x}-1) \quad (6)$$

for $0<x<\xi$ and $u(x)\equiv 0$ for $\xi\leqslant x\leqslant X$. Continuity of u at ξ implies that

$$g(\xi)\equiv k(1-\beta)\,\xi\int_0^\xi\left(\frac{t}{\xi}\right)^{1/(1-\beta)}e^{(1-\beta)\xi t}\,dt-ke^{(1-\beta)\xi^2}=-(k+1). \quad (7)$$

We claim that this equation can have no more than one solution ξ. It will be enough to show that $g'\leqslant 0$. We have

$$g'(\xi)=-k\beta\int_0^\xi\left(\frac{t}{\xi}\right)^{1/(1-\beta)}e^{(1-\beta)\xi t}\,dt-k\xi(1-\beta)\,e^{(1-\beta)\xi^2}$$
$$+k\xi(1-\beta)^2\int_0^\xi t\left(\frac{t}{\xi}\right)^{1/(1-\beta)}e^{(1-\beta)\xi t}\,dt.$$

The sum of the last two terms of $g'(\xi)$ can be written as

$$k\xi(1-\beta)\left(\frac{1-\beta}{\xi}\int_0^\xi t^2\left(\frac{t}{\xi}\right)^{\beta/(1-\beta)}e^{(1-\beta)\xi t}\,dt-e^{(1-\beta)\xi^2}\right)$$
$$\leqslant k\xi(1-\beta)\left(\frac{1-\beta}{\xi}\int_0^\xi t^2e^{(1-\beta)\xi t}\,dt-e^{(1-\beta)\xi^2}\right)$$
$$=-\frac{2k}{(1-\beta)\xi^3}\,((1-\beta)\,\xi^2e^{(1-\beta)\xi^2}-e^{(1-\beta)\xi^2}+1)\leqslant 0$$

since $(z-1)\,e^z+1\geqslant 0$ for $z\geqslant 0$. Thus $g'\leqslant 0$. Furthermore, application of l'Hopital's rule shows that $g(0)=-k$ and that the first term of $g'(\xi)$ tends to $-\infty$ as $\xi\to\infty$; we conclude that (7) always has a unique solution which may not, however, satisfy $\xi<X$. Conversely, if (7) has a solution $\xi<X$ then the preceding argument shows that (3)–(5) has a solution with a dead

core on $[\xi, X]$. Moreover, we see that a solution with a dead core will exist for X sufficiently large, since (7) is independent of X.

Case 2. $u(x) > 0$ on $[0, X)$. Proceeding in the same fashion we find that $v = (1-\beta)X$ and that

$$u'(x) + (1-\beta)\, Xu(x) = (1-\beta)\, X\left(k\left(\frac{x}{X}\right)^{1/(1-\beta)} + C_1\right), \tag{8}$$

whence

$$e^{(1-\beta)Xx}\, u(x) = 1 + k(1-\beta)X \int_0^x \left(\frac{t}{X}\right)^{1/(1-\beta)} \times e^{(1-\beta)Xt}\, dt + C_1\left(e^{(1-\beta)Xx} - 1\right);$$

$u(X) = 0$ implies that

$$C_1 = -\frac{1 + k(1-\beta)X \int_0^X (t/X)^{1/(1-\beta)}\, e^{(1-\beta)Xt}\, dt}{e^{(1-\beta)X^2} - 1}.$$

Thus we have determined formally a solution of the boundary value problem; the only question is whether or not $u > 0$ holds on $[0, X)$. If the root ξ of (7) satisfies $\xi > X$ then, since $g' \leqslant 0$, it must be that $g(X) > -(k+1)$. $C_1 < -k$ follows, and (8) yields

$$u'(x) + (1-\beta)\, Xu(x) < -(1-\beta)\, Xk\left(1 - \left(\frac{x}{X}\right)^{1/(1-\beta)}\right) \leqslant 0.$$

Therefore $u(x) = 0$ implies that $u'(x) < 0$, and it follows that the solution above is positive on $[0, X)$.

Our considerations show that there can be at most one solution with a dead core and at most one without a dead core. Suppose that one of each were to exist and let u denote the solution without a dead core. Since the root ξ of (7) satisfies $\xi < X$, we must have $g(X) < -(k+1)$. But then we have that

$$C_1 = -\frac{1 + g(X) + ke^{(1-\beta)X^2}}{e^{(1-\beta)X^2} - 1} > -k.$$

From (8) evaluated at X we obtain that $u'(X) > 0$, an impossibility. Hence the solution of (3)–(5) is unique, and it has a dead core if X is sufficiently large.

Existence for the Problem in a Finite Domain

This section is devoted to proving

THEOREM 1. *For each $X > 0$ the problem (1)–(3) has at least one nonnegative solution.*

As usual in arguments based on the topological transversality theorem, we study a related one-parameter family of problems

$$u''(x) + vu'(x) = [\lambda k\, |u(x)|^\alpha\, w^\beta(x) + (1-\lambda)\, kw^\beta(x)] \operatorname{sgn} u(x) \qquad (1_\lambda)$$

$$vw'(x) = \lambda\, |u(x)|^\alpha\, w^\beta(x) + (1-\lambda)\, w^\beta(x) \qquad (2_\lambda)$$

subject to the same boundary conditions (3), for $\lambda \in [0, 1]$. By a solution we understand a triple (u, v, w) with $u \in C^2(0, X) \cap C[0, X]$, $w \in C^1(0, X) \cap C[0, X]$, and $v \in R$ such that $w \geqslant 0$, $v > 0$ and (1_λ)–(2_λ), (3) are satisfied. In fact, $u \geqslant 0$ will also hold, so a solution of (1_1)–(2_1), (3) will be a nonnegative solution of (1)–(3). The advantage of the new formulation is that, even for $\lambda = 1$, it has only nonnegative solutions, as will be shown.

Let us first examine the special problem $\lambda = 0$. Integration of (2_0) and use of $w(0) = 0$ yields

$$vw^{1-\beta}(x) = (1-\beta)x$$

since we assume that $\beta < 1$. Evaluating this expression at X yields $v = (1-\beta)X$, so we obtain that $w(x) = (x/X)^{1/(1-\beta)}$. Then u must satisfy

$$u''(x) + (1-\beta)\, Xu'(x) = k(x/X)^{\beta/(1-\beta)} \operatorname{sgn} u(x). \qquad (9)$$

Were u anywhere negative, there would exist a point $\xi \in (0, X)$ such that $u(\xi) < 0$, $u'(\xi) = 0$, $u''(\xi) \geqslant 0$. But (9) shows that $u''(\xi) < 0$, a contradiction. Since (9) implies that u cannot have a positive local maximum on $(0, X)$, we must have $u' \leqslant 0$. Hence $u \geqslant 0$ must satisfy

$$u''(x) + (1-\beta)\, Xu'(x) = \begin{cases} k(x/X)^{\beta/(1-\beta)}, & 0 < x < \xi, \\ 0, & \xi \leqslant x \leqslant X, \end{cases} \quad u(0) = 1,\ u(X) = 0;$$

where $\xi \in (0, X]$ is the leftmost zero of u. This problem is explicitly and uniquely solvable by the argument of the preceding section. Thus we conclude that (1_0)–(2_0), (3) has a unique solution provided $\beta < 1$.

Let (u, v, w) be a solution of (1_λ)–(2_λ), (3). From (2_λ) we obtain that $w' \geqslant 0$, and so $0 \leqslant w \leqslant 1$. Suppose now that u had a strict local maximum at some $\xi \in (0, 1)$. Then on some nontrivial interval $(\xi, \zeta]$ we would have

$u(x) < u(\xi)$. Since $u'(\xi) = 0$ we would have from (2_λ) that, for $x \in (\xi, \zeta]$, $u'(x) + v[u(x) - u(\xi)] \geqslant 0$, implying that $u'(x) > 0$, an absurdity. Similarly, u cannot have a negative minimum. Hence u is monotone nonincreasing and $0 \leqslant u(x) \leqslant 1$.

Subtracting k times (2_λ) from (1_λ), integrating, and using the fact that $u \geqslant 0$ and the boundary conditions at 0 leads to

$$u'(x) + vu(x) - kvw(x) \leqslant u'(0) + v; \tag{10}$$

evaluation of (10) at X yields

$$(k+1)v \geqslant u'(X) - u'(0). \tag{11}$$

Integration of (2_λ) and use of the boundary conditions on w yields

$$v = \lambda \int_0^X u^\alpha(t)\, w^\beta(t)\, dt + (1-\lambda) \int_0^X w^\beta(t)\, dt,$$

from which we obtain the bound $v \leqslant X$. Since $(u' + vu)' \geqslant 0$, we have for $0 \leqslant \xi < x \leqslant 1$ that $u'(x) - u'(\xi) \geqslant v(u(\xi) - u(x)) \geqslant 0$; i.e., u' is nondecreasing. Letting $\xi = 0$ we obtain $u'(x) \geqslant u'(0)$; from (11) we then obtain $u'(x) \geqslant u'(X) - (k+1)v$. Geometrical considerations show that $u'(X) \geqslant -1/X$; thus

$$0 \geqslant u'(x) \geqslant -(k+1)\, X - \frac{1}{X} \equiv -M.$$

Thus we have established a priori bounds on u, u', w, and v independent of $\lambda \in [0, 1]$.

On suitable function spaces set

$$\|u\|_0 = \max_{x \in [0, X]} |u(x)|,$$

$$\|u\|_1 = \max\left(\|u\|_0, \frac{1}{M} \|u'\|_0 \right);$$

let B denote the Banach space $C^1[0, X] \times R \times C[0, X]$ equipped with the norm $|||(u, v, w)||| \equiv \max(\|u\|_1, |v|/X, \|w\|_0)$ for $(u, v, w) \in B$. Note that any solution of (1_λ)–(2_λ), (3) satisfies $|||(u, v, w)||| \leqslant 1$. Define K by

$$K = \{(u, v, w) \in B : u \geqslant 0, u(0) = 1, u(X) = 0; v \geqslant 0;$$
$$w \geqslant 0, w(0) = 0, w(X) = 1\};$$

then K is convex. Finally, for any $\delta > 0$ define

$$U = \{(u, v, w) \in K : |||(u, v, w)||| < 1 + \delta\};$$

then U is a relatively open subset of K and no solution of (1_λ)–(2_λ), (3) lies on the boundary of U.

For $\lambda \in [0, 1]$ we define a map N_λ on $\bar{U}$ by $N_\lambda : (u, v, w) \mapsto (\hat{u}, \hat{v}, \hat{w})$, where

$$\hat{v} = (1-\beta)\left[\lambda \int_0^X u^\alpha(t)\,dt + (1-\lambda)X\right], \tag{12}$$

$$\hat{v}\hat{w}^{1-\beta}(x) = (1-\beta)\left[\lambda \int_0^x u^\alpha(t)\,dt + (1-\lambda)x\right], \tag{13}$$

$$\begin{aligned} \hat{u}'(x) + \hat{v}\hat{u}(x) = \lambda k \int_0^x u^\alpha(t)\, \hat{w}^\beta(t) \operatorname{sgn} \hat{u}(t)\, dt \\ + (1-\lambda) k \int_0^x \hat{w}^\beta(t) \operatorname{sgn} \hat{u}(t)\, dt \\ + \hat{u}'(0) + \hat{v}, \qquad \hat{u}(X) = 0. \end{aligned} \tag{14}$$

For the moment we put off showing that N_λ is in fact well defined. In (14) $\hat{u}'(0)$ is to be regarded as a parameter to be determined so as to satisfy the boundary condition. Since $u(0) = 1$, $\hat{v} > 0$ and $0 < \hat{w}(x) \leqslant 1$ on $(0, X]$. We claim that $0 \leqslant \hat{u}(x) \leqslant 1$ holds also. To see this, suppose $\hat{u}$ has a positive strict local maximum at $\xi \in (0, X)$. Then on some nontrivial interval $(\xi, \zeta]$ we have $0 < \hat{u}(x) < \hat{u}(\xi)$ holding. Therefore the right-hand side of (14) is continuously differentiable on $(\xi, \zeta]$ and we have

$$(\hat{u}'(x) + \hat{v}\hat{u}(x))' = \lambda k u^\alpha(x)\, \hat{w}^\beta(x) + (1-\lambda)\, k\hat{w}^\beta(x) \geqslant 0$$

there. Hence

$$\hat{u}'(x) \geqslant \hat{v}(\hat{u}(\xi) - \hat{u}(x)) > 0,$$

an obvious impossibility. In the same way, $\hat{u}$ cannot have a negative local minimum. It follows that $0 \leqslant \hat{u}(x) \leqslant 1$ on $[0, X]$ and that $\hat{u}'(x) \leqslant 0$ there.

In view of the foregoing, the right-hand sides of (13)–(14) are continuously differentiable, except for at most one point ξ, where $\hat{u}(\xi) = 0$ with $\hat{u}(x) > 0$ for $x < \xi$, and we have, except at ξ, that

$$\hat{u}''(x) + \hat{v}\hat{u}'(x) = \lambda k u^\alpha(x)\, \hat{w}^\beta(x) \operatorname{sgn} \hat{u}(x) + (1-\lambda)\, k\hat{w}^\beta(x) \operatorname{sgn} \hat{u}(x) \tag{15}$$

$$\hat{v}\hat{w}'(x) = \lambda u^\alpha(x)\, \hat{w}^\beta(x) + (1-\lambda)\, \hat{w}^\beta(x) \tag{16}$$

$$\hat{u}(0) = \hat{w}(1) = 1, \qquad \hat{u}(1) = \hat{w}(0) = 0. \tag{17}$$

Conversely, a piecewise-C^2 solution of (15)–(17) satisfies (12)–(14). Thus

N_λ: $\bar{U} \to K$. Since fixed points of N_λ in $\bar{U}$ are precisely the solutions of (1_λ)–(2_λ), (3), we have that N_λ is fixed-point free on the boundary of U.

We have not yet shown that N_λ is well defined; i.e., that $\hat{u}$ is unique. Since the right-hand side of (15) is not necessarily continuous, this is not obvious. But this follows from

LEMMA 1. *Let* $y \in C^1(0, X) \cap C[0, X]$ *satisfy*

$$y''(x) + cy'(x) = h(x) \operatorname{sgn} y(x), \qquad y(0) = 1,\ y(X) = 0,$$

almost everywhere on $(0, X)$, *where h is continuous and nonnegative, and c is a positive constant. Then y is unique.*

Proof. Suppose y and $\hat{y}$ are both solutions and set $z = y - \hat{y}$. We may suppose that $\xi \in (0, X]$ and $\zeta \in [\xi, X]$ are the first points at which $\hat{y}$ and y, respectively, vanish. We have shown above that y and $\hat{y}$ are nonincreasing and nonnegative. Then z satisfies

$$z''(x) + cz'(x) = h(x) \cdot \begin{cases} 0, & 0 \leqslant x < \xi, \\ 1, & \xi \leqslant x < \zeta, \\ 0, & \zeta \leqslant x \leqslant X, \end{cases} \qquad z(0) = z(1) = 0.$$

Straightforward but somewhat tedious calculations show that this problem has a solution in $C^1(0, 1)$ only if $\xi = \zeta$, and then the solution is $z \equiv 0$. ∎

Set

$$h(x) \equiv \lambda k u^\alpha(x)\, \hat{w}^\beta(x) + (1 - \lambda)\, k \hat{w}^\beta(x), \qquad H(x) \equiv \int_0^x h(t)\, dt.$$

Then, as far to the right of 0 as $\hat{u}$ is positive we have $\hat{u}''(x) + \hat{v}\hat{u}'(x) = h(x)$, whence, on integration,

$$\hat{u}'(x) + \hat{v}\hat{u}(x) = H(x) + \hat{u}'(0) + \hat{v}. \tag{18}$$

It follows on a further integration from 0 to x that

$$\hat{u}(x) = e^{-\hat{v}x} \int_0^x e^{\hat{v}s} H(s)\, ds + \frac{\hat{u}'(0)}{\hat{v}} [1 - e^{-\hat{v}x}] + 1. \tag{19}$$

Now suppose there exists a least $\xi \in (0, X)$ such that $\hat{u}(\xi) = 0$. Then also $\hat{u}'(\xi) = 0$ and $\hat{u} \equiv 0$ on $[\xi, X]$. From (18) above evaluated at ξ we obtain that

$$\hat{u}'(0) = -H(\xi) - \hat{v}, \tag{20}$$

so the vanishing of (19) yields

$$0 = g(\xi) \equiv \int_0^\xi e^{\hat{v}s} H(s)\, ds - \frac{H(\xi)}{\hat{v}} (e^{\hat{v}\xi} - 1) + 1. \tag{21}$$

Since

$$g'(z) = -\frac{h(z)}{\hat{v}} (e^{\hat{v}z} - 1) \leqslant 0,$$

Eq. (21) has at most one root ξ, or else the set of solutions constitutes an interval. Conversely, let $\xi \in (0, X)$ be the least root of (21) and define $\hat{u}'(0)$ by (20). Then $\hat{u}$ given by (19) on $[0, \xi]$ and $\hat{u} \equiv 0$ on $[\xi, X]$ is the unique (by Lemma 1) solution of (15), (17). Thus we have a representation of $\hat{u}$ for this case.

Suppose next that there is no $\xi \in (0, X)$ such that $g(\xi) = 0$; i.e., suppose that $g(X) > 0$. Then the previous argument shows that $\hat{u}(x) > 0$ must hold for $0 \leqslant x \leqslant X$, and thus that (19) holds there. Evaluating (19) in the limit as $x \to X$ and using the boundary condition $\hat{u}(X) = 0$, we obtain that

$$\hat{u}'(0) = -\hat{v} \frac{e^{\hat{v}X} + \int_0^X e^{\hat{v}s} H(s)\, ds}{e^{\hat{v}X} - 1}. \tag{22}$$

Therefore in this case $\hat{u}$ is given on $[0, X]$ by (19) with the value of $\hat{u}'(0)$ specified in (22).

If (21) has a least root ξ in $(0, X)$, set $\Xi = \xi$; otherwise set $\Xi = X$. Then $\hat{u}$ is given by (19), with $\hat{u}'(0)$ from (20) or (22), on $[0, \Xi]$, and $\hat{u}(x) \equiv 0$ on $[\Xi, X]$. Since $\sup |u'| \leqslant M(1+\delta)$ we have that $u(x) \geqslant 1 - M(1+\delta)x$ on $[0, 1/M(1+\delta)]$; it follows from (12) that there exists a $V > 0$ independent of λ and $u \in \bar{U}$ such that

$$\hat{v} \geqslant (1-\beta) \left[\lambda \int_0^{1/M(1+\delta)} (1 - M(1+\delta)t)^\alpha\, dt + (1-\lambda) X \right] \geqslant V.$$

It is now evident that $\hat{v}$ and $\hat{w}$ depend continuously on u and λ. It follows from (21) and the subsequent equation that g and g' depend continuously on u and λ. Observe that (20) and (22) are equivalent when X is the least root of (21). If $g'(\xi) < 0$ when $g(\xi) = 0$ so the root of (21) is unique or if $g(X) > 0$, then the continuous dependence of Ξ and $\hat{u}'(0)$ on u and λ follows readily. Suppose that $g(z) = 0$ for $\xi \leqslant z \leqslant \xi + \delta$ for some $\delta > 0$ and $\xi < X$; then $h(z) = 0$ and $H(z)$ is a constant there as well. It follows from (20) that $\hat{u}'(0) = -H(z) - \hat{v}$ for $\xi \leqslant z \leqslant \xi + \delta$ and thus that $\hat{u}'(0)$ is a continuous function of u and λ in this case as well, although Ξ is not. From (19) we obtain that $\hat{u}$ depends continuously on u and λ in the sup norm and (18) then implies that $\hat{u}'$ is also continuous in u and λ. We conclude that N_λ is a continuous homotopy of $\bar{U}$ into K.

We must show that $\bigcup_{\lambda \in [0,1]} N_\lambda(\bar{U})$ is contained in a compact subset of K. Since from (12) we have $\hat{v} \leqslant X(1+(1+\delta)^\alpha)$, $\hat{v}$ lies in the interval $[V, X(1+(1+\delta)^\alpha)]$. $\hat{w}$ satisfies $0 \leqslant \hat{w} \leqslant 1$ for $(u, w, v) \in \bar{U}$; from (16) we have $0 \leqslant \hat{w}'(x) \leqslant (1/V)((1+\delta)^\alpha + 1)$. Thus the Arzela–Ascoli theorem guarantees that $\hat{w}$ lies in a compact subset of $C[0, X]$, independent of λ and of $(u, v, w) \in \bar{U}$. Now the function h is bounded by $k[(1+\delta)^\alpha + 1]$ and H by $kX[(1+\delta)^\alpha + 1]$. From (20) and (22) we have that $|\hat{u}'(0)|$ is bounded by

$$X(1+(1+\delta)^\alpha) \max\left(k+1, \frac{1 + kX^2(1+(1+\delta)^\alpha)}{1 - e^{-VX}}\right).$$

We already know that $0 \leqslant \hat{u}(x) \leqslant 1$. It follows from (18) that $\hat{u}'(x)$ is also uniformly bounded; thus $\{\hat{u}\}_{(u,v,w) \in \bar{U}}$ is uniformly bounded and equicontinuous. If $0 \leqslant r < t \leqslant \Xi$, then from the equicontinuity of $\hat{u}$ and H it follows that

$$\begin{aligned} |\hat{u}'(t) - \hat{u}'(r)| &\leqslant \hat{v}\, |\hat{u}(t) - \hat{u}(r)| + |H(t) - H(r)| \\ &\leqslant C_1\, |t - r| \end{aligned}$$

for some constant C_1, independent of $(u, v, w) \in \bar{U}$ and $\lambda \in [0, 1]$. If $0 \leqslant r < \Xi \leqslant t \leqslant X$, then

$$|\hat{u}'(t) - \hat{u}'(r)| = |\hat{u}'(\Xi) - \hat{u}'(r)| \leqslant C_1\, |\Xi - r| \leqslant C_1\, |t - r|;$$

the equicontinuity of $\hat{u}'$ follows. Therefore the Arzela–Ascoli theorem asserts that $\hat{u}$ lies in a precompact subset of $\{C^1[0, X], \|\cdot\|_1\}$ for $(u, v, w) \in \bar{U}$ and $\lambda \in [0, 1]$. By the Tychonoff product theorem, N_λ is a compact homotopy.

As we have already seen, the map N_0 is a constant map to an interior point of U; therefore it is essential [4]. The topological transversality theorem guarantees that N_1 is also essential and so has a fixed point in U. This fixed point (u, v, w) is a solution of (1_1)–(2_1), (3) and, since $u \geqslant 0$, also of (1)–(3). ∎

Uniqueness

Suppose (u_1, v_1, w_1) and (u_2, v_2, w_2) are two solutions of (1)–(3) with $v_1 < v_2$. Dividing (2) by $w^\beta(x)$ and integrating from 0 to X yields

$$v_1 = (1-\beta) \int_0^X u_1^\alpha(x)\, dx < (1-\beta) \int_0^X u_2^\alpha(x)\, dx = v_2;$$

hence there must exist some point in $(0, X)$ at which $u_1 - u_2 < 0$. Suppose $\xi < \zeta$ are two points in $(0, X)$ such that $(u_1 - u_2)(\xi) = (u_1 - u_2)(\zeta) = 0$, $(u_1 - u_2)'(\xi) \leqslant 0$, and $(u_1 - u_2)'(\zeta) \geqslant 0$. Then from (1)–(2) we obtain

$$(u_1 - u_2)'' + v_1(u_1 - u_2)' + (v_1 - v_2)u_2' = k(v_1 w_1 - v_2 w_2)';$$

integration from ξ to ζ yields

$$\begin{aligned} 0 &\leqslant (u_1 - u_2)'(\zeta) - (u_1 - u_2)'(\xi) + (v_1 - v_2)(u_2(\zeta) - u_2(\xi)) \\ &= k[(v_1 w_1 - v_2 w_2)(\zeta) - (v_1 w_1 - v_2 w_2)(\xi)]. \end{aligned} \tag{23}$$

If we may take $\xi = 0$, $\zeta = X$, then (23) and the boundary conditions (3) imply that $(v_1 - v_2) \geqslant 0$, a contradiction. Suppose now that $u_1 - u_2 > 0$ on the interval $(0, \xi)$ with ξ as above. Since $v_1 w_1' w_1^{-\beta} = u_1^\alpha > u_2^\alpha = v_2 w_2' w_2^{-\beta}$ there, we have $v_1 w_1^{1-\beta}(\xi) > v_2 w_2^{1-\beta}(\xi)$ on integration. Since $v_1 < v_2$, we must have $w_1(\xi) > w_2(\xi)$, so that $(v_1 w_1 - v_2 w_2)(\xi) > 0$. If we may take $\zeta = X$ above, then (23) yields

$$0 < v_2 - v_1 \leqslant (v_2 w_2 - v_1 w_1)(\xi),$$

again a contradiction. Suppose next that $u_1 - u_2 > 0$ on the interval (ζ, X) with ζ as above. Integrating $v_1 w_1' w_1^{-\beta} > v_2 w_2' w_2^{-\beta}$ over this interval leads us to

$$v_1[1 - \omega_1^{1-\beta}(\zeta)] > v_2[1 - w_2^{1-\beta}(\zeta)] > v_1[1 - w_2^{1-\beta}(\zeta)]$$

since $w_i \leqslant 1$, or $0 > v_1 - v_2 = v_1 w_1^{1-\beta}(\zeta) - v_2 w_2^{1-\beta}(\zeta)$ and $w_1(\zeta) < w_2(\zeta)$. It follows that $v_1 w_1(\zeta) - v_2 w_2(\zeta) < 0$. If we may take $\xi = 0$, then (23) yields $v_1 w_1(\zeta) - v_2 w_2(\zeta) \geqslant 0$, a contradiction. If $u_1 - u_2 > 0$ on both $(0, \xi)$ and (ζ, X), then a combination of these arguments leads to a similar contradiction. Finally, if $u_1 - u_2$ oscillates near either 0 or X, then passage to the limit in (23) as $\xi \downarrow 0$ or as $\zeta \uparrow X$ along suitable sequences leads to the contradiction $v_1 - v_2 \geqslant 0$. It follows that $v_1 \not< v_2$, and hence by symmetry that $v_1 = v_2$.

To finish showing uniqueness we shall need the following lemma.

LEMMA 2. *Let $0 < \beta < 1$. Then the solution (u, w) of the initial value problem*

$$u'' + vu' = ku^\alpha w^\beta, \qquad vw' = u^\alpha w^\beta,$$

$$u(0) = 1, \qquad u'(0) = \gamma, \qquad w(0) = 0$$

with $w > 0$ for $x > 0$ is unique at least to the first zero of u.

Proof. From the equation for w we have

$$w(x) = \left(\frac{1-\beta}{v}\int_0^x u^\alpha(s)\,ds\right)^{1/(1-\beta)}$$

as far to right of zero as $u(x)>0$. Thus the equation for u can be written in the form

$$u''(x) + vu'(x) = C_1 \frac{d}{dx}\left[\left(\int_0^x u^\alpha(s)\,ds\right)^{1/(1-\beta)}\right],$$

where we write C_1 for $k(1-\beta)^{1/(1-\beta)}v^{-\beta/(1-\beta)}$. Hence

$$u'(x) + vu(x) = \gamma + v + C_1\left(\int_0^x u^\alpha(s)\,ds\right)^{1/(1-\beta)}$$

for some constant γ; a further integration yields

$$u(x) = e^{-vx} + \left(\frac{\gamma}{v}+1\right)\left(1-e^{-vx}\right)$$
$$+ C_1\int_0^x e^{-v(x-t)}\left(\int_0^t u^\alpha(s)\,ds\right)^{1/(1-\beta)} dt.$$

If (u_1, w_1) and (u_2, w_2) are two solutions of the initial value problem, then as far as both u_1 and u_2 are positive we have that

$$|u_1-u_2|\,(x) \leqslant C_1\int_0^x \left|\left(\int_0^t u_1^\alpha(s)\,ds\right)^{1/(1-\beta)} - \left(\int_0^t u_2^\alpha(s)\,ds\right)^{1/(1-\beta)}\right| dt$$
$$\leqslant C_2\int_0^x\int_0^t |u_1^\alpha(s)-u_2^\alpha(s)|\,ds\,dt$$
$$= C_2\int_0^x (x-s)\,|u_1^\alpha-u_2^\alpha|\,(s)\,ds$$

because $1/(1-\beta)>1$, so the function $z^{1/(1-\beta)}$ is locally Lipschitz. As far as both u_1 and u_2 are positive, z^α is also locally Lipschitz, so we obtain that

$$|u_1-u_2|\,(x) \leqslant C_3\int_0^x (x-s)\,|u_1-u_2|\,(s)\,ds;$$

whence Gronwall's lemma implies that $u_1 \equiv u_2$ as far as both are positive. ∎

We return to showing that u and w are unique. Let (u_1, v, w_1) and (u_2, v, w_2) be solutions of (1)–(3). If $(u_1 - u_2)'(0) = 0$, then Lemma 2 and the known properties of solutions shows that $u_1 \equiv u_2$ on $[0, X]$ and hence that $w_1 \equiv w_2$. Suppose that $(u_1 - u_2)'(0) < 0$; then there must exist $\xi \in (0, X)$ such that $(u_1 - u_2)'(\xi) = 0$, $(u_1 - u_2)''(\xi) \geqslant 0$, and $(u_1 - u_2)(x) < 0$ for $x \in (0, \xi]$. Since $u_1 - u_2$ satisfies the differential equation

$$(u_1 - u_2)'' + v(u_1 - u_2)' - kw_1^\beta(u_1^\alpha - u_2^\alpha) = ku_2^\alpha(w_1^\beta - w_2^\beta),$$

we conclude that $w_1(\xi) > w_2(\xi)$. However, from

$$\frac{vw_1^{1-\beta}(\xi)}{1-\beta} = \int_0^\xi u_1^\alpha(s)\, ds < \int_0^\xi u_2^\alpha(s)\, ds = \frac{vw_2^{1-\beta}(\xi)}{1-\beta}$$

we arrive at the contradiction $w_1(\xi) < w_2(\xi)$. It follows that u and w are unique.

Remark on Monotonicity. A portion of the argument above can be modified easily to show that the velocity v is a nondecreasing function of interval length X. Indeed, for $i = 1, 2$ let (u_i, v_i, w_i) be the solution of (1)–(3) on the interval $(0, X_i)$ and let $X_1 > X_2$. Then (u_1, v_1, w_1) is the solution on $(0, X_2)$ of

$$u'' + vu' = ku^\alpha w^\beta, \quad vw' = u^\alpha w^\beta,$$

$$u(0) = 1, \qquad w(0) = 0, \qquad u(X_2) = \gamma, \qquad w(X_2) = \delta,$$

where $\gamma \equiv u_1(X_2) \in [0, 1)$ and $\delta \equiv w_1(X_2) \in (0, 1]$. A repeat of the first paragraph of the uniqueness proof when (u_1, v_1, w_1) satisfies this problem shows that $v_1 < v_2$ cannot happen.

Remark on Efficiency. The efficiency of the process may be defined as the fraction of the reactant of concentration u absorbed by the rod that ultimately enters into the chemical reaction. A measure of this is provided by $|u'(0) - u'(X)|$. From (11) we see that this is proportional to v, and thus, by the remark above, the process is more efficient the larger the domain.

Existence of a Dead Core for $0 < \alpha < 1$ and Large X

Let (u, v, w) be the solution of (1)–(3). Then $u'' + vu' \geqslant 0$, so by a standard comparison theorem $u(x) \leqslant z(x)$ where z is the solution of $z'' + vz' = 0$, $z(0) = 1$, $z(X) = 0$. Thus

$$u(x) \leqslant \frac{e^{-vx} - e^{-vX}}{1 - e^{-vX}} \equiv \frac{e^{-vx} - e^{-\zeta}}{1 - e^{-\zeta}}.$$

Now the right-hand side is an increasing function of ζ, so we obtain that $u(x) \leqslant e^{-vx}$. We use this inequality first to obtain an upper bound on v and a lower bound on w. Integrating the inequality $vw'w^{-\beta} \leqslant e^{-\alpha vx}$ from x to X, we obtain easily that

$$w^{1-\beta}(x) \geqslant 1 - \frac{1-\beta}{\alpha v^2} e^{-\alpha vx}, \qquad 0 \leqslant x \leqslant X;$$

evaluation at $x = 0$ in particular yields

$$v \leqslant \sqrt{(1-\beta)/\alpha},$$

an estimate independent of X. Since in this section we shall be concerned only with X sufficiently large, we assume henceforth that $X \geqslant 1$. The inequality $1-(1-\beta)\, e^{-\alpha vx}/(\alpha v^2) \geqslant \frac{1}{2}$ is equivalent to $2 \leqslant \alpha v^2 e^{\alpha vx}/(1-\beta)$. Since v is a nondecreasing function of X, if this inequality holds for v_1, the velocity corresponding to $X = 1$, it will hold for any larger v, and hence any $X \geqslant x$ as well. Solving, we see that $w^{1-\beta}(x) \geqslant \frac{1}{2}$ for

$$x \geqslant x_1 \equiv \frac{1}{\alpha v_1} \ln \left(\frac{2(1-\beta)}{\alpha v_1^2} \right)$$

and $X \geqslant x$. Note that x_1 is independent of X.

Using the fact that $u' \leqslant 0$, for $x_1 \leqslant x \leqslant X$ we have that

$$u'' \geqslant Cu^{\alpha},$$

where we set $C = k2^{-\beta/(1-\beta)}$. Integrating $u'u'' \leqslant Cu^{\alpha}u'$ from $x \in [x_1, X)$ to X we obtain that

$$u'(x)^2 \geqslant \frac{2C}{\alpha+1} u^{\alpha+1}(x),$$

whence

$$-u^{-(\alpha+1)/2}(x)\, u'(x) \geqslant \sqrt{2C/(\alpha+1)}$$

if there is no dead core, that is, if $u(x) > 0$ on $[0, X)$. A further integration from x_1 to X yields, for $\alpha < 1$,

$$u^{(1-\alpha)/2}(x_1) \geqslant (1-\alpha)\sqrt{C/2(\alpha+1)}(X - x_1).$$

Since the left-hand side is bounded by one and since x_1 is independent of X, this is impossible for X large. We have shown that, if $0 < \alpha < 1$, then a dead core (in u) is present for sufficiently large X. Of course, if $u \equiv 0$ on some $[\zeta, X]$, then $w \equiv 1$ there.

Existence and Uniqueness on the Semi-infinite Interval

We are concerned with the Eqs. (1)–(2) together with the boundary conditions

$$u(0)=1, \qquad \lim_{x\to\infty} u(x)=0, \qquad w(0)=0, \qquad \lim_{x\to\infty} w(x)=1. \tag{24}$$

Of course, if (1)–(3) for some X has a solution with a dead core, then (1)–(2), (24) clearly has a solution. Thus, in view of the result of the preceding section, we need be concerned solely with the case $\alpha \geqslant 1$ while establishing existence. Throughout this section we make free use of earlier results and notation.

We need a bound on $|u'(x)|$, i.e., on $|u'(0)|$, for the solution of (1)–(3). We have the obvious inequality,

$$u''+vu'=ku^{\alpha}w^{\beta}\leqslant ke^{-\alpha v x}.$$

Then $u(x)\geqslant y(x)$, where y is the solution of

$$y''+vy'=ke^{-\alpha v x}, \qquad y(0)=1, \qquad y(X)=0,$$

and, in particular, $0\geqslant u'(0)\geqslant y'(0)$. Calculation yields for $\alpha>1$ that

$$y'(0)=-\frac{k}{(\alpha-1)v}-\frac{\alpha(\alpha-1)v^2-k(1-e^{-\alpha v X})}{\alpha(\alpha-1)\,v(1-e^{-vX})}.$$

Now the right-hand side has a finite limit as $X\to\infty$ and therefore $|y'(0)|$ has a finite upper bound for $(v, X)\in[v_1, \sqrt{(1-\beta)/\alpha}]\times[1,\infty)$. Let $M_1(\alpha)$ denote such a bound; then we have $|u'(0)|\leqslant M_1(\alpha)$ for $\alpha>1$. For $\alpha=1$ a similar calculation yields

$$y'(0)=-\frac{k}{v}-\frac{v+k-kXe^{-vX}}{1-e^{-vX}},$$

so that $|y'(0)|$ is again bounded (say by $M_1(1)$) for $1\leqslant X<\infty$. From (1) we obtain directly the existence of a constant $M_2(\alpha)$ such that $|u''(x)|\leqslant M_2(\alpha)$ for $0\leqslant x\leqslant X$ and $1\leqslant X<\infty$.

Let (u_X, v_X, w_X) denote the solution of (1)–(3) for $X\in[1,\infty)$. We have shown that $0\leqslant u_X(x)\leqslant 1$, $|u_X'(x)|\leqslant M_1(\alpha)$, $|u_X''(x)|\leqslant M_2(\alpha)$, $v_1\leqslant v_X\leqslant \sqrt{(1-\beta)/\alpha}$, $0\leqslant w_X(x)\leqslant 1$, and, from (2), $|w_X'(x)|\leqslant 1/v_1$, on $[0, X]$. Fix any $Z>1$ and consider on $[0, Z]$ the families of functions $\{u_X\}_{X>Z}$, $\{u_X'\}_{X>Z}$, and $\{w_X\}_{X>Z}$. Our estimates show that each of these families is uniformly bounded and equicontinuous; hence, by the Arzela–Ascoli theorem, there exist continuous functions u, u' w on $[0, Z]$ such that for some increasing, unbounded subsequence $\{X_i\}$,

$$u_{X_i} \to u, \qquad u'_{X_i} \to u', \qquad w_{X_i} \to w \tag{25}$$

uniformly on $[0, Z]$. By the usual diagonalization process, we may assume that u, u', and w are continuous on $[0, \infty)$ and that (25) holds uniformly on each compact subset of $[0, \infty)$; then $v_{X_i} \uparrow v$ for some constant v. From (1)–(2) we have that

$$u'_X(x) + v_X u_X(x) = u'_X(0) + v_X + k \int_0^x u_X^\alpha(t)\, w_X^\beta(t)\, dt,$$

$$v_X w_X(x) = \int_0^x u_X^\alpha(t)\, w_X^\beta(t)\, dt$$

on $[0, Z]$; passage to the limit through the subsequence $\{X_i\}$ yields

$$u'(x) + vu(x) = u'(0) + v + k \int_0^x u^\alpha(t)\, w^\beta(t)\, dt,$$

$$vw(x) = \int_0^x u^\alpha(t)\, w^\beta(t)\, dt$$

there. It follows that (u, v, w) is a solution of (1)–(2) on each $[0, Z]$ and hence on $[0, \infty)$. Of course, we have $u(0) = 1$, $w(0) = 0$. From the inequality $u_{X_i}(x) \leqslant e^{-v_{X_i} x} \leqslant e^{-v_1 x}$ we obtain that $\lim_{x \to \infty} u(x) = 0$.

While proving the existence of a dead core for $\alpha < 1$ we showed that for all $\alpha > 0$ there exists a number x_1 independent of $X \geqslant 1$ such that $x_1 \leqslant x \leqslant X$ implies $w_X(x) \geqslant \frac{1}{2}$. In the same way, for each integer n there exists an x_{n-1} independent of X sufficiently large such that $w_X(x) \geqslant 1 - 1/n$ for $x_{n-1} \leqslant x \leqslant X$. From this it follows that $\lim_{x \to \infty} w(x) = 1$. Thus (u, v, w) satisfies (1)–(2), (24).

In much the same way as for the problem on the finite interval, the vital estimates $0 \leqslant u \leqslant 1$, $0 \leqslant w \leqslant 1$, $u' \leqslant 0$ can be seen to hold for the problem on the semi-infinite interval. The proof of uniqueness on a finite interval can now be modified slightly to show that there is only one solution to the problem (1)–(2), (24).

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